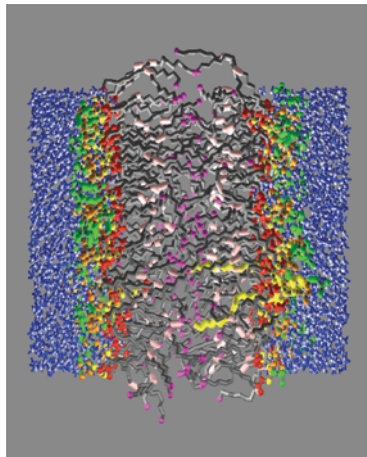


Molecular Dynamics Simulations

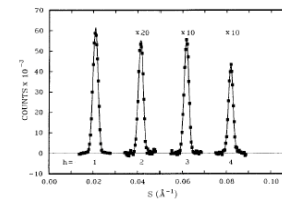
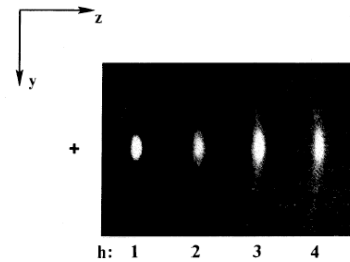
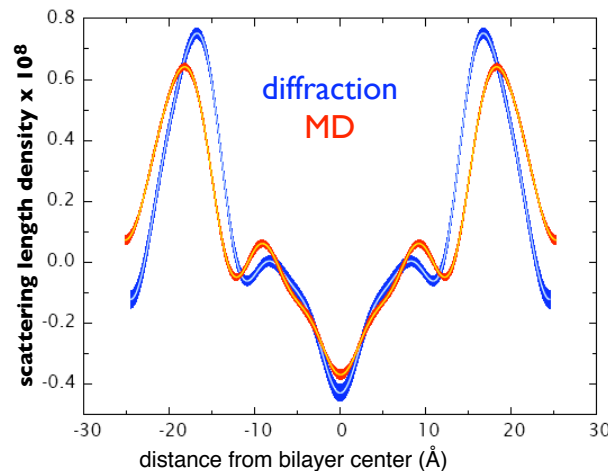
MD simulations & diffraction experiments:
teaming up to refine disordered structures in 3D



MD simulations:
all-atom phase trajectories

- 3D details to 1D structure
- predictions stimulate new experiments

$$\Delta(z) = \Delta_0 + \frac{2}{d} \sum_{h=1}^{h_{\max}} F(h) \cos \frac{\sum_{\sum} \sum \frac{\Delta h z}{d} \sum_{\sum}}$$



diffraction:
structure factor amplitudes

- validation & refinement of simulation methods
- data for restraint potentials

Benz, Castro-Roman, Tobias & White, BJ (2005)